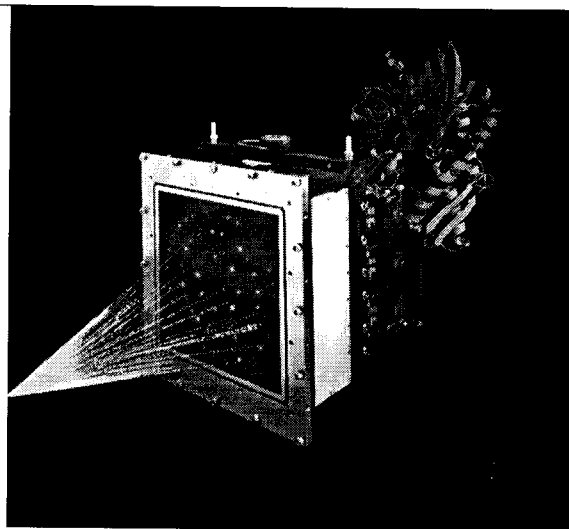


CCD (CHARGE-COUPLED DEVICE) DETECTORS FOR CRYSTALLOGRAPHY



Argonne National Laboratory

Electronics and Computer Science

Steven N. Snaday

snaday@anl.gov

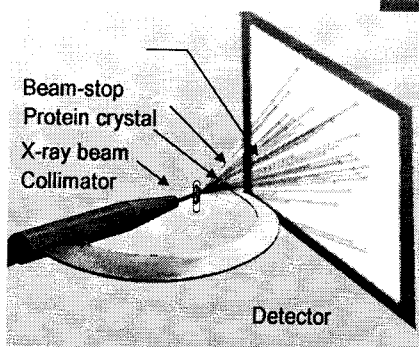
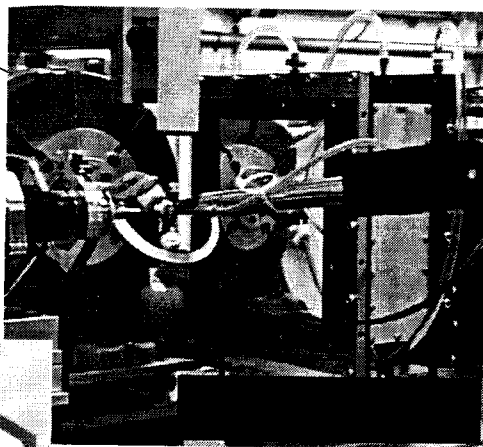
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CCD (Charge-Coupled Device) Detectors for Crystallography

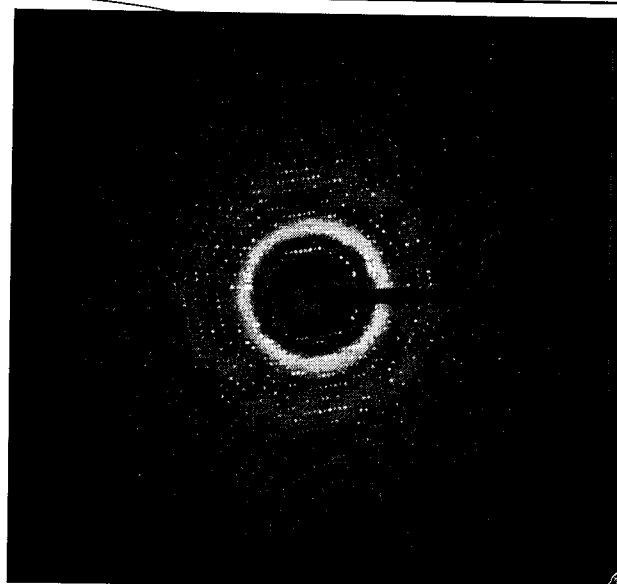
- Detector requirements for macromolecular diffraction measurements
- Overview of CCD detector technology
- Quantitative analysis of performance parameters
- Future directions of CCD detector development

Protein Crystallography Setup (APS-SBC 19BM)



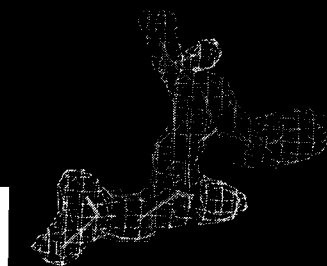
Typical parameters:

X-ray energy range: 6-20keV
X-ray intensity (main beam): 10^{13} XPh/s
crystal volume: 10^{-3} mm³
crystal to detector distance: 70 - 900mm
exposure time: 0.1s - 20s
number of frames / data set: 100 - 1000



MAD: Multiple-wavelength Anomalous Dispersion measurement at 2 - 4 different energy

electron density map,
combined with the
corresponding phase of the
molecule.



CCD Detectors for protein crystallography:

Integrating type detectors

Advantages:

- virtually unlimited count-rate capability
- very high pixel count ($> 10^6$ pixels)
- simple readout
- timing capability

Disadvantages:

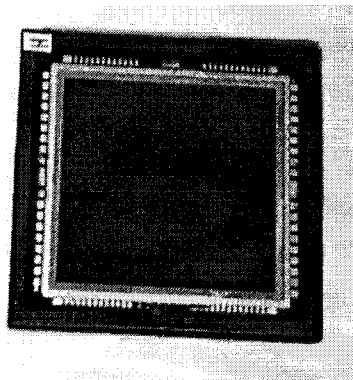
- readout and dark current noise introduces errors at low intensities
- dead during readout

Does the data quality improve significantly, by using counting detectors ?

- Dynamic range: **>20,000** at $10^5/\text{sec}$ XPh/s count-rate in CCD detectors
In counting detectors this would require < 5 pps/pixel false pulses
- The scattered X-ray background is the dominant noise source usually ...
- At high count rates, accuracy is limited in CCD detectors to $\sim 0.3\text{--}0.5\%$.

Charge Coupled Device is a solid-state imager:

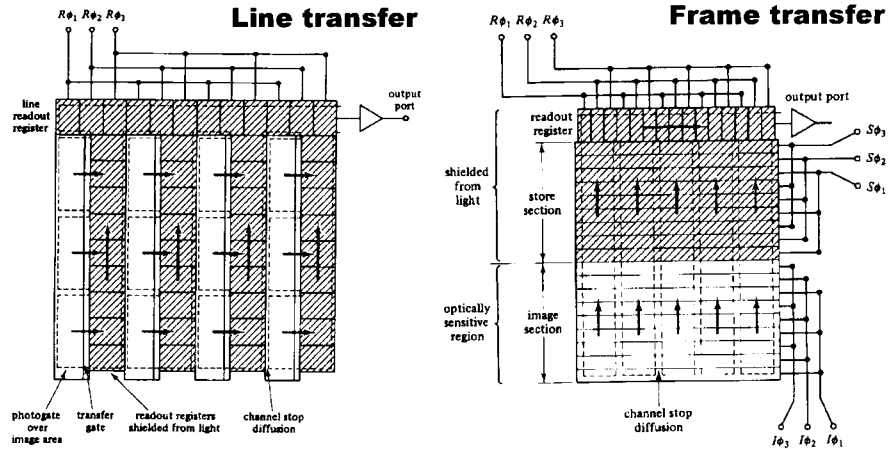
- converts light to electron-hole pairs
- stores charge pattern in picture elements (pixels)
- shifts charge packets in pixels to output(s)
- converts charge to voltage on output



Thompson-CSF (now ATMEL)
2048 x 2048 pixels
Pixel size: 13 x 13 μm
Imaging area: 28 mm x 28 mm

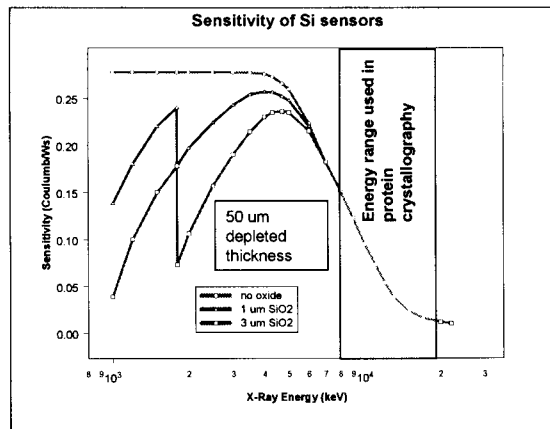
Readout structures:

- line transfer
- frame transfer
- full frame
- single/multiple readout amplifiers



Direct detection of X-ray by CCD's:

Low sensitivity (8keV-20keV)
Radiation damage
Too high gain
etc.



Indirect detection:
X-ray
↓
Visible light
↓
electrons

CCD Detector technologies

Single Fiber-Optic Taper Detectors

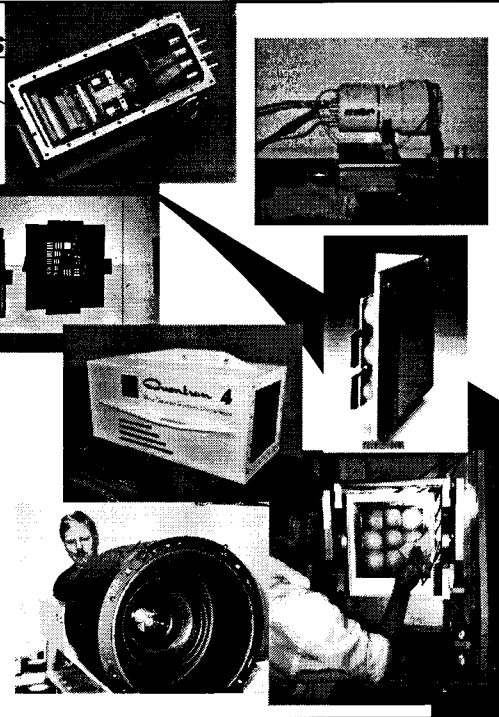
Fiber-Optic Faceplate Detectors

Multiple (Mosaic) Fiber-Optic Taper Detectors

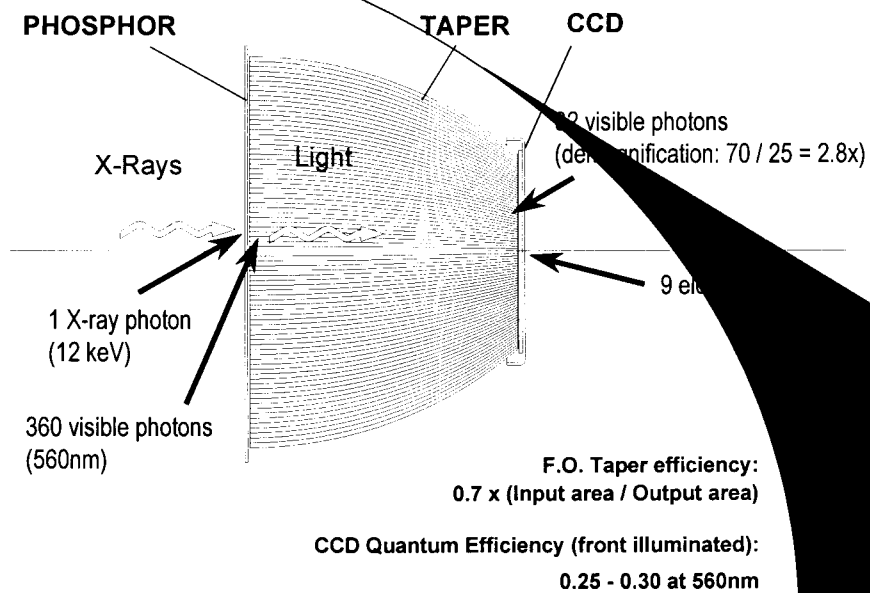
Lens Coupled Detectors

Direct X-ray detection with CCD's

Time-resolved imaging with CCD's



Demagnification by fiber-optic taper



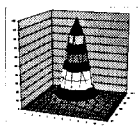
GENERAL DETECTOR REQUIREMENTS

- Very large dynamic range > 10,000 / pixel
 - low noise < 20 electrons rms / pixel (combined noise)
 - high saturation level > 350,000 electrons / pixel
- Large area > 200 mm x 200 mm
- High sensitivity > 5 electrons / XPh
- Very high "count rate" capability > 10⁶ electrons / pixel / s
- Good linearity < 0.5% deviation from linearity
- High stability < 0.5% gain drift, < 0.1% baseline drift
- Short readout time < 2 seconds / frame

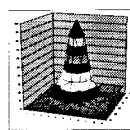
Comparing detector parameters

Meaningful characterization of detector performance should be based on how the quality of the collected data is affected by the detector parameters?

Input:
Typical diffraction peak on the
detector face



Output:
Observed diffraction peak



Quantitative comparison of the

- conversion gain, noise and saturation level
- sensitive area (size) of the the detector

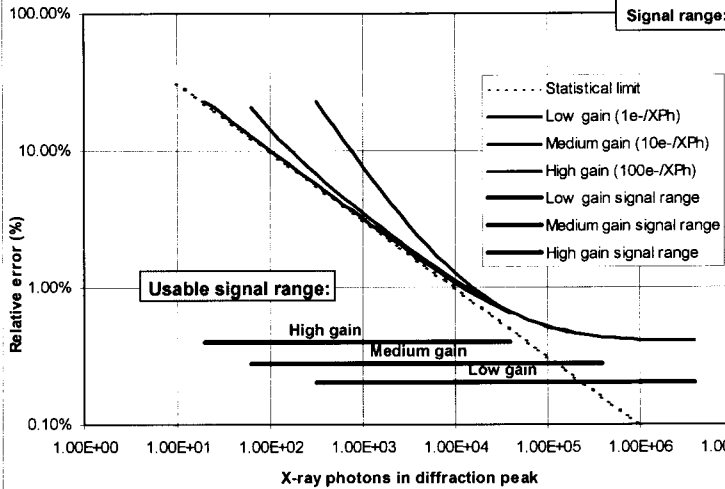
Conversion Gain:

Number of photoelectrons generated in the CCD pixels by 1 X-ray photon (typically at 12 keV)

Conditions:

Sample size: 150 μm x 150 μm
 Integration: 5x5 pixels
 Integral / peak pixel value: 10x
 Dark and read noise / pixel: 20 e- rms
 Pixel saturation: 400,000 e-
 Signal range: 20% error to saturation

Error vs. detector gain



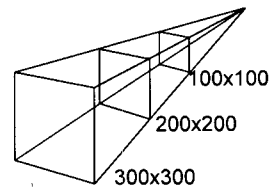
Conversion gain of available detectors:

ADSC Q210: 3.4 e-/XPh
 SBC-2: 8 e-/XPh
 Bruker lens: 7e-/XPh?
 (0.65e-/XPh w. same phosphor, front illum. CCD, corner..)

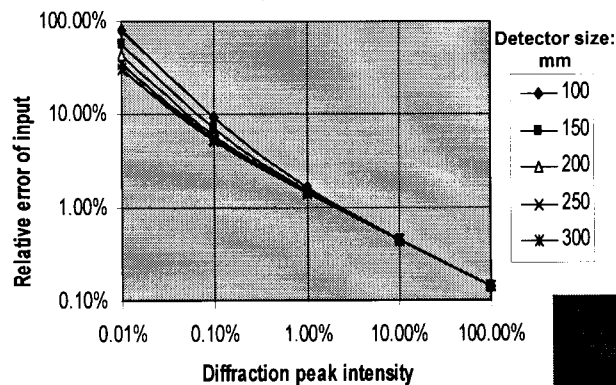
Size of detector area (1):

1. Background suppression:

- diffuse X-ray background is proportional with d^2



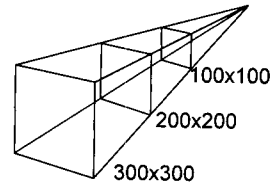
Effect of background vs. detector size



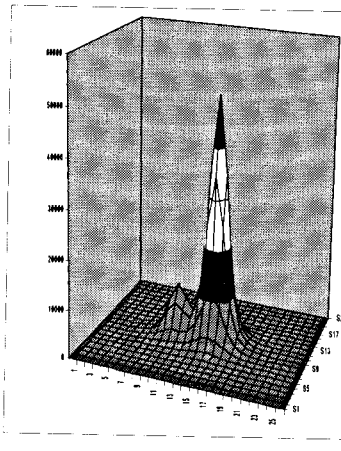
Size of detector area (2):

2. Resolution

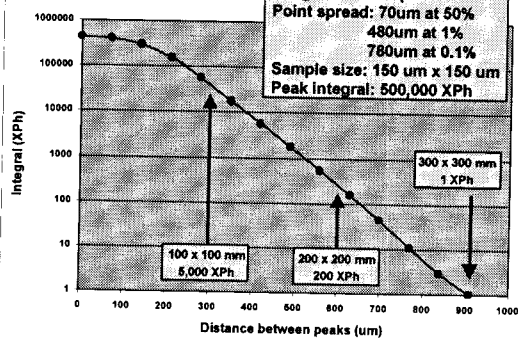
Resolving power: closely placed diffraction peaks should be resolvable, even with large samples



Spot size is defined primarily by the sample size and phosphor resolution...



"Crosstalk" of peaks



Future trends in CCD detector technology

- Large area mosaic detectors based on fiber-optic taper demagnifiers (4x4)
- Lens coupled systems
- Fast readout imaging detectors

Development required:

- Phosphor / scintillator technology
- Multiple output, high resolution CCD's
- Lower priced, very large area CCD's

- Amorphous silicon based detectors ("Flat panel detectors")



Conclusion:

- CCD technology is a well established technology for large area detectors
- Further improvements are possible
- Specialized CCD detectors (e.g. very fast readout cameras for time resolved applications) can be developed for future applications



Thank you for your attention...

